Algorithms of "cloud approximation" for nonconvex sets in a finitedimensional space Gornov A.Yu.

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Applications areas

- reachable set of controllable system
- trajectory of dynamical system
- estimation of the local extrema regions of the function
- multicriteria optimization
- data analysis

Problems

- phase estimation
- nonlocal optimal control methods
- search for a global function extremum
- variational inequalities
- impacts of normalization

"Cloud approximation" Term

- irregular grid
- randomized mesh
- stochastic grid
- set of points

- ..

The optimal control problem with box constraints

$$\dot{x} = f(x, u, t)$$

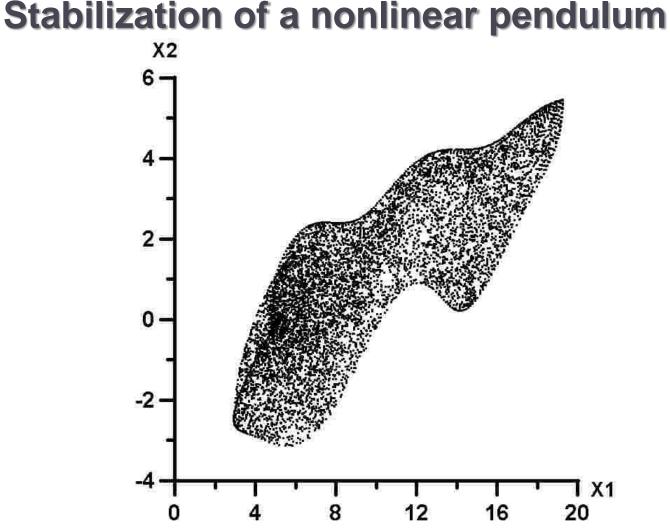
$$x(t_0) = x^0, \quad t \in T = [t_0, t_1]$$

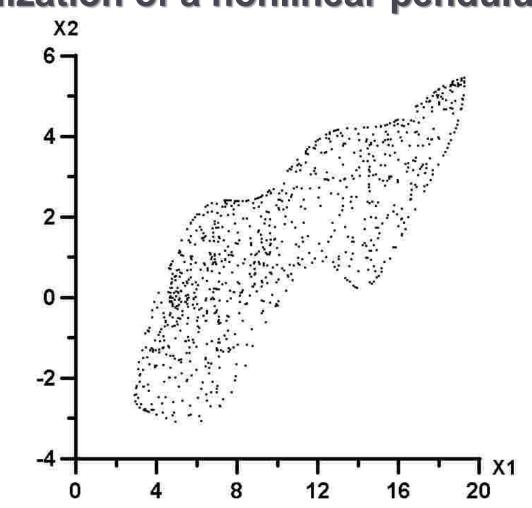
$u(t) \in U = \{ u \in R^r : \underline{u}_i \le u_i \le \overline{u}_i \}$

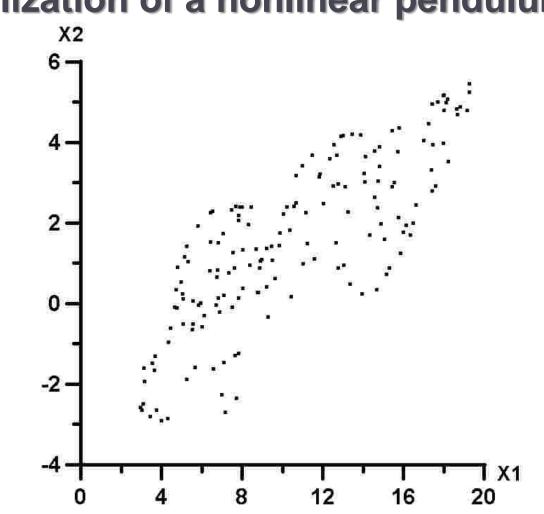
$I(u) = \varphi(x(t_1)) \rightarrow \min$

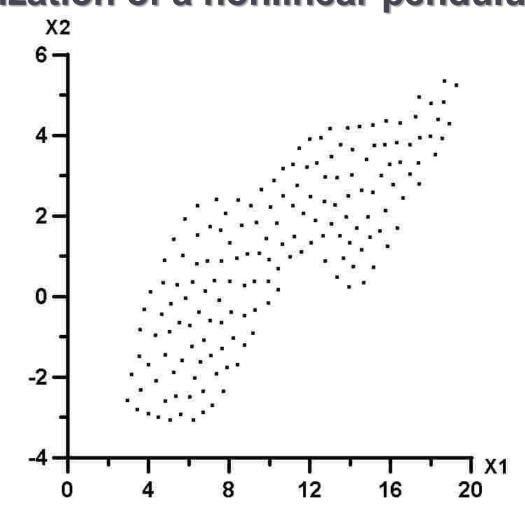
 $\dot{x}_1 = x_2$ $\dot{x}_{2} = u_{1} - \sin x_{1}$ $|u_1(t)| \leq 1$ $t \in [0, 5]$ x(0) = (5, 0) $I(u) = x_1^2(5) + x_2^2(5) \rightarrow \min$

The approximation problem of the reachable set









A common approach input-output system

- uniform approximation of input parameters
- processing of multiple output parameters

Approach to the construction of algorithms

- only scalable basic operations (Euclidean norms, *L*₁-norms, ...)
- no more than subquadratic computing schemes
- visualization

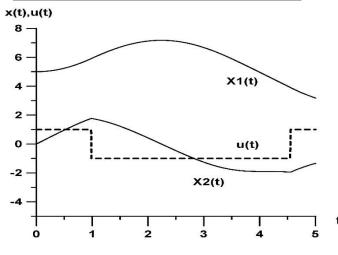
Test problems 01

$$\dot{x}_1 = x_2$$

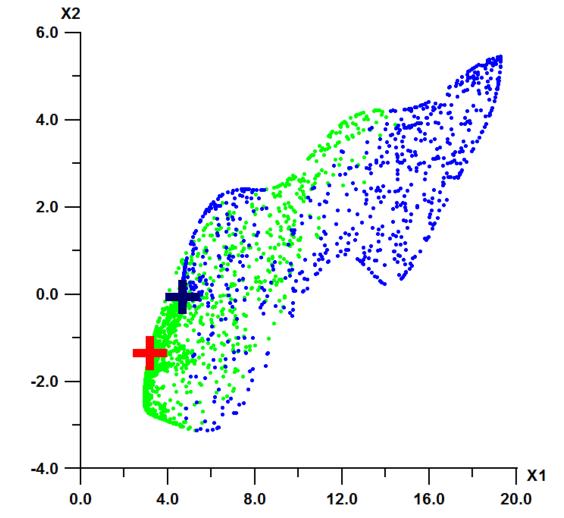
$$\dot{x}_2 = u_1 - \sin x_1$$

Iteration – 1000, CPU time is 7591 sec., Number of solved Cauchy problems – 186015

N	Functional	Value
1	1.190817e+01	0.457
2	2.182900e+01	0.543



$$x(0) = (5, 0) \quad t \in [0, 5] \quad | u_1(t) | \le 1$$
$$I(u) = x_1^2(5) + x_2^2(5) \to \min$$



The global optimization problem Approach

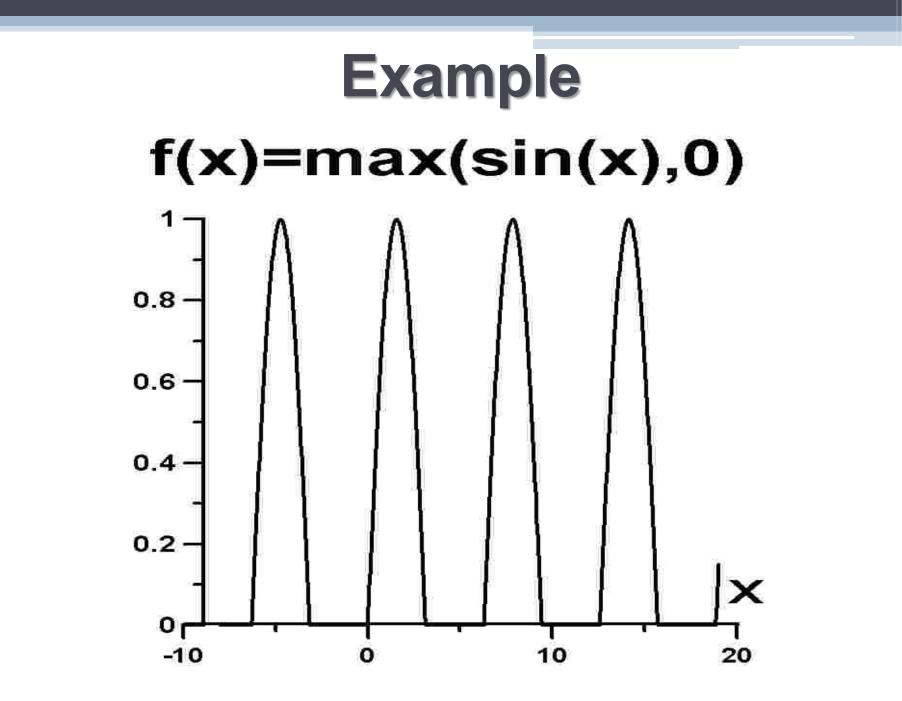
- Identification and evaluation of local extremum areas
- decomposition of the original problem into subtasks with the "small" reachable sets

The global optimization problem formulation $f(x) - > \min, x \in X$

 $f(x) \rightarrow \min_{x_i} x_j \leq x \leq x_o$

 $x \in X = \{ x_l \le x \le x_g \} : f(x) = f^*$

 $X^* \in X : \forall x \in X^* f(x) = f^*$



Classification of optimization problems by the number of extrema

- "Low extremes" 2-5 extrema
- "Medium-extreme" 5-30 extrema
- "Multiextremal" 30-"many extrema"
- with a multivalued solution infinitely many extrema

Example

Optimization of Atomic Molecular Potentials Morse Potential

- the number of variables = 3 * number of atoms
- the number of local extrema grows as an exponent of the atoms number
- with the number of atoms = 147, the estimate of the number of local extrema is $10^{**}60$
- officially registered record is 240 atoms. The number of extrema > 10**100?

Cambridge Cluster Database

Classification of optimization problems by structure of extrema

- several extrema with different values of the function
- several extrema with the same value of the function
- a set of solutions with the same value of the function
- sets of solutions with different values of the function

Global optimization problems and hopes

- the problem of the volume ratio of the search set and the possibilities of searching, the resource of probes
- the problem dimension is 100, box [0,1], volume 1
- the problem dimension is 100, box [0,2], volume 2**100=(1024)**10 = 1.26*10**30

Global optimization problems and hopes

 in order to solve the global optimization problem, one must be able to solve only two problems:

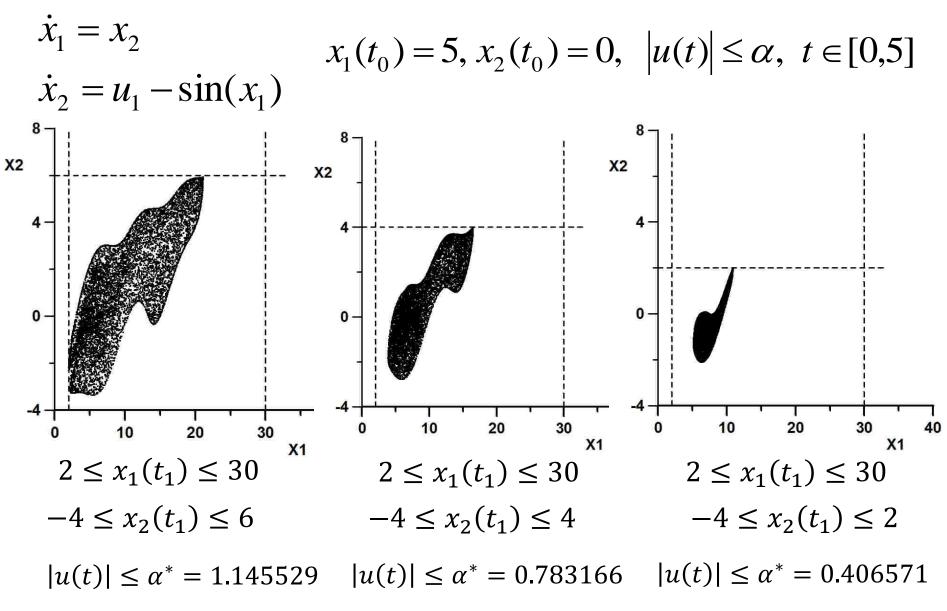
 find one point in the region of the global extremum attraction;
find the minimum of unimodal function

Open problems Control of trajectory beams

- Control in conditions of indeterminacy (in the system both control and perturbation)
- The problem of formulating the "nuclear problem"
- Example: impacts of normalization

$$u^{k}(t) + \delta u^{k}(t), \left\| \delta u^{k}(t) \right\| \leq \Delta$$

Test problem 02



Popular approximative constructions

- "boxes"
- spheres
- ellipsoids
- meshes ("cloud")
- parallelotopes
- simplexes
- ovaloids

^{- .}

"Cloud approximation"

Algorithms for realization of "set-theoretic" operations

- association
- intersection
- addition
- convexication
- delineation
- boundary approximation
- evaluation of the "diameter"
- estimation of "spread"
- estimate the volume of the set

"Cloud approximation" Algorithm for addition constructing

- outlining the original "cloud" with a box
- generation of test points from a box
- fixation in the "cloud"-addition of test points far from the points of the original "cloud"

"Cloud approximation" Algorithm for addition constructing 0 20 12th International Conference on Intelligent Data Processing: Theory and Applications»

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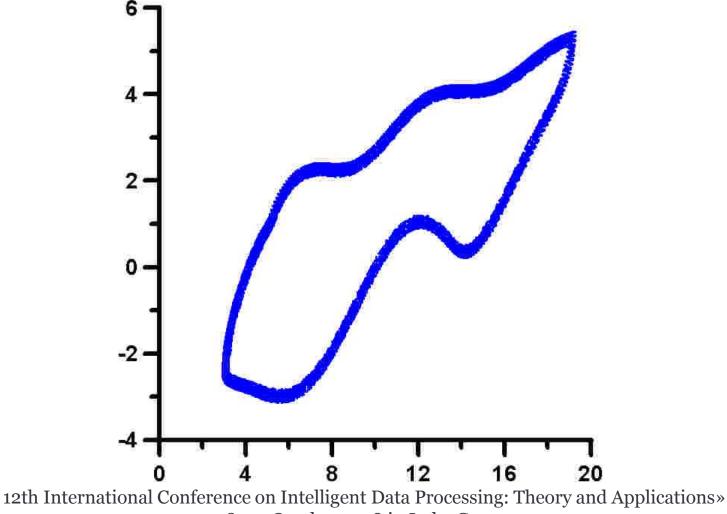
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"Cloud approximation" Algorithm for the boundary approximation

- the construction of a "cloud"-addition
- removal of points close to the points of the original "cloud"

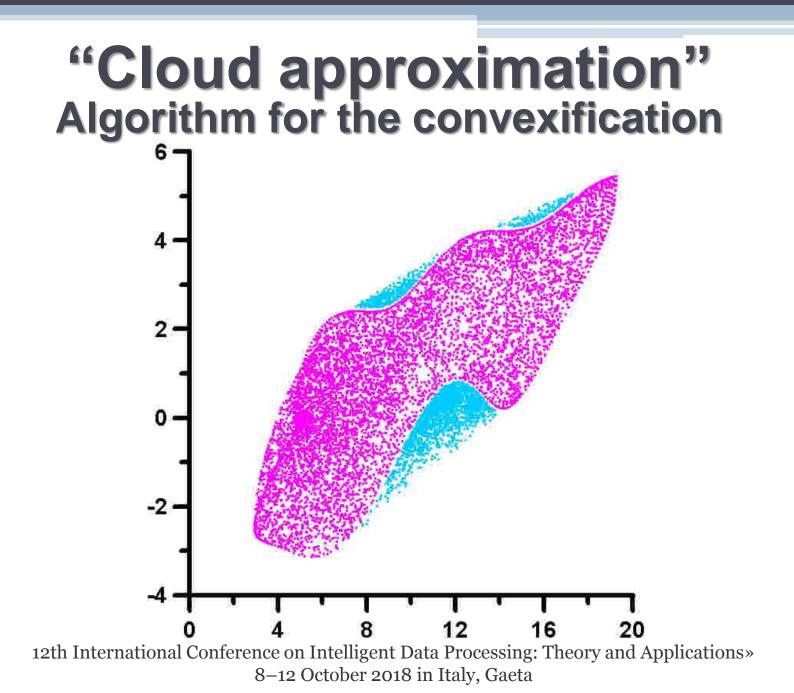
"Cloud approximation" Algorithm for the boundary approximation



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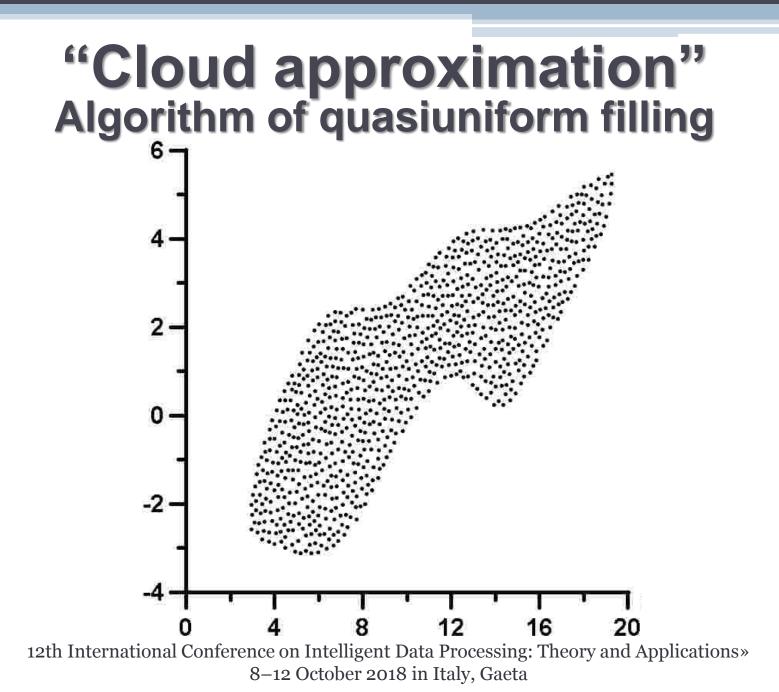
"Cloud approximation" Algorithm for the convexification

- selecting pairs of points from the original "cloud"
- generation of test points on the connecting segments
- selection of test points, fixation of the points from the original "cloud" that do not fall in the its neighborhoods



"Cloud approximation" Algorithm of quasiuniform filling

- generation a start "cloud" from one point
- generation of test points
- selection of test points, fixation of points not including in the neighborhood of a point of the already existing "cloud"



"Cloud approximation" The algorithm for estimating the volume of the set ("Archimedes' algorithm")

- outlining the "cloud" with the box
- quasiuniform filling of the "cloud"
- quasiuniform filling of the contouring box
- volume estimation through the ratio of the points number in the set and the box approximations

Estimation of the cluster volume Archimedes' algorithm

- fixe *R* radius of the test sphere
- "the enclosing" box is constructed
- calculate *N* the number of cluster elements lying at least *R* from each other
- calculate *M* the number of disjoint spheres of radius *R* that fill the enclosing box
- cluster volume estimation is equal the box volume * *M* / *N*

The FOREL clustering method "Formal Element"

- convergence is proved in a finite number of steps
- strong dependence on the choice of the first point
- relatively low productivity
- close to linear computational complexity
- 1) Zagoruiko N.G., Yolkina V.N., Lbov G.S. Algorithms for detecting empirical regularities. Novosibirsk: Science, 1985. 999 p. (In Russian).
- Zagoruiko N.G. Applied methods of data and knowledge analysis. Novosibirsk: IM SB RAS, 1999. – 270 p. – ISBN 5-86134-060-9.

Software OPTCON-SV (version 0.5)

- algorithms for estimating the record value of the function
- algorithms for generation of "cloud approximation"
- FOREL algorithm for clustering
- tools for research, fixation and visualization of the clusters

Software OPTCON-SV Algorithms for "clouds" generation

- stochastic approximation algorithm
- algorithm of approximation with a search "along the Polak"
- approximation algorithm with Hooke-Jeeves search
- algorithm of deterministic approximation for the function of two variables

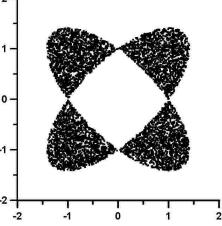
Software OPTCON-SV Tools

- table of distances between the centers of the clusters
- sphere chart of the cluster
- coordinate cluster chart
- cluster estimation algorithm of Archimedes
- the lower bound of the function value on the cluster

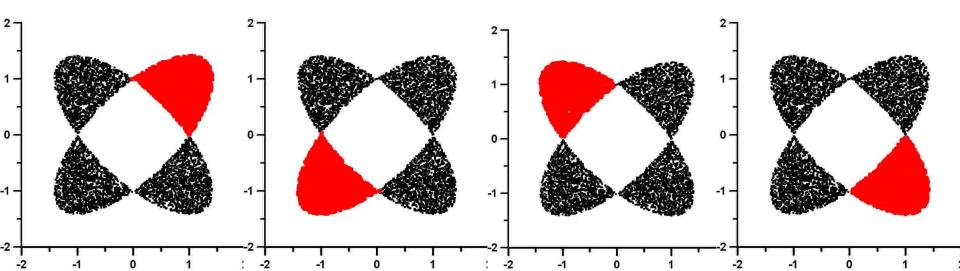
Test problem 03

calculation by the method of stochastic approximation, 1 min. of CPU time, about 600,000 samples, found 6714 points

$$f(x_1, x_2) = (x_1 - 1)^2 (x_1 + 1)^2 + (x_2 - 1)^2 (x_2 + 1)^2$$



$$f(x_1, x_2) \le 1$$



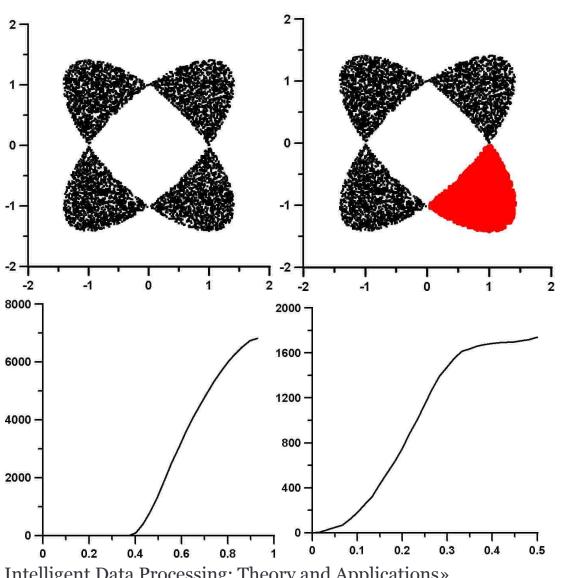
"Cloud approximation" What do we want and what is obtained with the help of "prequadratic" algorithms

- find an estimate of the record value of the function
- find the estimate of the location region of the global extremum
- reduce the volume of the search box
- exclude unpromising areas
- increase the probability of finding a global extremum
- bypass the hard gullies

Sphere chart of the cluster

The number of cluster points falling into a sphere of increasing radius with center at the center of gravity of the cluster

Table of distances between cluster centers



Conclusions

- simple algorithms give a good result
- it is possible to evaluate sets with complex geometry
- there is no strict limitation in dimension
- there is potential for parallelization

- "Cloud" approximations can be a useful tool

Thank you for attention!

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